

# Simulation of four-body interaction in a nuclear magnetic resonance quantum information processor \*

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Four-body interaction plays an important role in many-body systems, and it can exhibit interesting phase transition behaviors. Historically it was the need to efficiently simulate quantum systems that lead the idea of a quantum computer. In this Letter, we report the experimental demonstration of a four-body interaction in a four-qubit nuclear magnetic resonance quantum information processor. The strongly modulating pulse is used to implement spin selective excitation. The results show a good agreement between theory and experiment.

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## I. INTRODUCTION

Quantum computers have advantages over the classical counterparts in simulating quantum systems [1] and solving some hard problems, such as factoring large number and searching unsorted databases [2]. Among the various candidates for implementing the large-scale quantum computer in the future and demonstrating quantum algorithms to corroborate existing theories, liquid nuclear magnetic resonance (NMR) has been proven a convenient and practical method to learn lessons for the other physical systems [3]. NMR quantum computer is an Ising-type computer [4] where two-body interactions take the form of  $\pi J_{ij} \sigma_z^i \sigma_z^j / 2$ , known as  $J$ -couplings in NMR, where  $\sigma_z^i$  denotes the Pauli matrix of the  $i$ -th spin, and  $J_{ij}$  denotes the strength of coupling between two spins.

There have been much interests in many-body interactions. Besides two-body interactions, many-body interactions are valuable sources for quantum information processors. For example, the three-spin interactions can speed up the quantum state transfer in the Heisenberg spin chain [5]. Four-body interactions have attracted much interests recently [6]. The systems with many-body interactions can exhibit interesting phase transition behaviors [6], such as quantum entanglement phase transitions [7]. The three spin-interactions in the spin chain can induce the quantum criticality that cannot be measured by concurrence, because three-spin interactions generate three-qubit entanglement [7]. Four-body interaction may play an important role in phase transition in some condensed matters [6].

Simulation of quantum system is one of main applications of future quantum computers. Practical factoring and searching applications of quantum computer usually require hundreds even thousands of qubits. But the simulation of quantum systems may require only a few dozens

of qubits. Thus simulating quantum systems may well be the first practical application of the early practical quantum computer. It is helpful now to study the simulations of quantum system with a few qubit quantum information processor, to locate problems and gather experiences, in particular the unitary operations and the extent of decoherence in existing apparatus. In fact, it has been successfully demonstrated that three-body interaction can be simulated very well in NMR quantum computers [5, 8]. It is a reasonable assumption that the four-spin interactions relate to four-qubit entanglement, which is still unclear for us currently. In this paper we focus on implementing the four-spin interactions in a NMR quantum computer. Our work is a valuable step in exploring quantum simulations, and also a crucial step for implementing the quantum phase transitions induced by four-body interactions and investigating the relation between the four-spin interactions and four-qubit entanglement experimentally.

## II. GENERATING FOUR-SPIN INTERACTIONS USING NMR

Our task is to decompose the four-spin evolution into a series of one-spin operations and  $J$ -couplings. The one-spin operations are realized by radio frequency pulses. The  $J$ -coupling evolution

$$U_{zz}(T) = e^{-i(\pi/2)J_{ij}T\sigma_z^i\sigma_z^j} \quad (1)$$

can be realized by standard NMR spin-echo techniques [9]. Under  $U_{zz}(T)$ ,  $\sigma_x^i$  evolves as

$$\sigma_x^i \xrightarrow{J_{ij}} \sigma_x^i \cos \theta + \sigma_y^i \sigma_z^j \sin \theta \quad (2)$$

where  $\theta = \pi J_{ij}t$ .

Through some calculations [10] one finds that the  $n$ -spin interaction can be decomposed as the  $(n-1)$ -spin

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interactions by iteration

$$\begin{aligned}
& e^{-i(\pi/2)J_{12}\dots T\sigma_z^1\sigma_z^2\dots\sigma_z^n} \\
&= e^{-i(\pi/4)\sigma_x^2}e^{-i(\pi/4)\sigma_z^1\sigma_z^2} \\
&\quad \times e^{-i(\pi/4)\sigma_y^2}e^{-i(\pi/2)J_{12}\dots T\sigma_z^2\dots\sigma_z^n} \\
&\quad \times e^{-i(\pi/4)\sigma_y^2}e^{-i(\pi/4)\sigma_z^1\sigma_z^2}e^{i(\pi/2)\sigma_y^2}e^{i(\pi/4)\sigma_x^2}. \quad (3)
\end{aligned}$$

By introducing

$$P_1(n) = e^{-i(\pi/4)\sigma_x^{n+1}}e^{-i(\pi/4)\sigma_z^n\sigma_z^{n+1}}e^{-i(\pi/4)\sigma_y^{n+1}}, \quad (4)$$

$$P_2(n) = e^{-i(\pi/4)\sigma_y^{n+1}}e^{-i(\pi/4)\sigma_z^n\sigma_z^{n+1}}e^{i(\pi/2)\sigma_y^{n+1}}e^{i(\pi/4)\sigma_x^{n+1}}. \quad (5)$$

Eq. (3) can be further expressed as

$$\begin{aligned}
& e^{-i(\pi/2)J_{12}\dots T\sigma_z^1\sigma_z^2\dots\sigma_z^n} = \\
& \prod_{l=1}^{n-2} P_1(l) e^{-i(\pi/2)J_{12}\dots T\sigma_z^{n-1}\sigma_z^n} \prod_{m=1}^{n-2} P_2(n-1-m). \quad (6)
\end{aligned}$$

From Eq. (6) one finds that the many-spin interaction can be decomposed into the operations that can be directly realized by NMR. When  $n = 4$  one obtains

$$\begin{aligned}
U_{zzzz}(T) &= e^{-i(\pi/2)J_{1234}T\sigma_z^1\sigma_z^2\sigma_z^3\sigma_z^4} \\
&= e^{-i(\pi/4)\sigma_x^2}e^{-i(\pi/4)\sigma_z^1\sigma_z^2}e^{-i(\pi/4)\sigma_y^2}e^{-i(\pi/4)\sigma_x^3} \\
&\quad \times e^{-i(\pi/4)\sigma_z^2\sigma_z^3}e^{-i(\pi/4)\sigma_y^3}e^{-i(\pi/2)J_{1234}T\sigma_z^3\sigma_z^4} \\
&\quad \times e^{-i(\pi/4)\sigma_y^3}e^{-i(\pi/4)\sigma_z^2\sigma_z^3}e^{i(\pi/2)\sigma_y^3}e^{i(\pi/4)\sigma_x^3} \\
&\quad \times e^{-i(\pi/4)\sigma_y^2}e^{-i(\pi/4)\sigma_z^1\sigma_z^2}e^{i(\pi/2)\sigma_y^2}e^{i(\pi/4)\sigma_x^2}, \quad (7)
\end{aligned}$$

where  $J_{1234}$  is the effective strength of the four-spin interaction. The above equation can also be represented as

$$\begin{aligned}
U_{zzzz}(T) &= e^{-i(\pi/4)\sigma_x^2}e^{-i(\pi/4)\sigma_z^1\sigma_z^2}e^{-i(\pi/4)\sigma_y^2}e^{-i(\pi/4)\sigma_x^2} \\
&\quad \times e^{-i(\pi/4)\sigma_z^2\sigma_z^3}e^{-i(\pi/4)\sigma_y^3}e^{-i(\pi/2)J_{1234}T\sigma_z^3\sigma_z^4}e^{i(\pi/4)\sigma_y^2} \\
&\quad \times e^{-i(\pi/2)\sigma_y^2}e^{-i(\pi/4)\sigma_z^2\sigma_z^3}e^{i(\pi/2)\sigma_y^2}e^{i(\pi/4)\sigma_x^2} \\
&\quad \times e^{-i(\pi/4)\sigma_y^2}e^{-i(\pi/4)\sigma_z^1\sigma_z^2}e^{i(\pi/2)\sigma_y^2}e^{i(\pi/4)\sigma_x^2}. \quad (8)
\end{aligned}$$

### III. IMPLEMENTATION

We use Carbon-13 labelled crotonic acid dissolved in  $D_2O$  as the sample. The chemical sketch of crotonic acid is shown as Fig. 1, where C1 - C4 are assigned as qubits 1 - 4, respectively. The protons are decoupled during the whole experiment. The experiments are implemented on

a Bruker DRX 500 MHz spectrometer. The temperature is controlled at 22 °C.

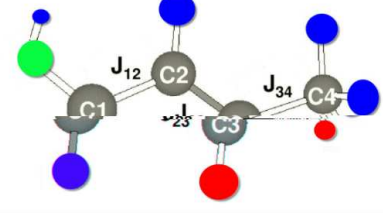


FIG. 1: (Color online) Molecule of crotonic acid. The blue spheres denote protons and the green spheres denote oxygens. The chemical shifts are  $\nu_1 = 21468.9$  Hz,  $\nu_2 = 15255.6$  Hz,  $\nu_3 = 18668.0$  Hz, and  $\nu_4 = 2190.4$  Hz. The  $J$  coupling constants are  $J_{12} = 72.4$  Hz,  $J_{13} = -1.3$  Hz,  $J_{14} = 7.0$  Hz,  $J_{23} = 70.3$  Hz,  $J_{24} = -1.6$  Hz, and  $J_{34} = 41.3$  Hz.

The Hamiltonian of the NMR system reads

$$H_{NMR} = -\pi \sum_{k=1}^4 \nu_k \sigma_z^k + \frac{1}{2} \pi \sum_{k < l} J_{kl} \sigma_z^k \sigma_z^l, \quad (9)$$

where  $\nu_1 - \nu_4$  are the resonance frequencies of C1 - C4. The coupled-spin evolution between two spins is denoted as

$$[\tau_{kl}] = e^{-i\frac{1}{2}\pi J_{kl}\tau\sigma_z^k\sigma_z^l}, \quad (10)$$

where  $k/l = 1, 2, 3, 4$ , and  $k \neq l$ .  $[\tau_{kl}]$  can be realized by averaging the coupling constants other than  $J_{kl}$  to zero [9]. The pulse sequence to implement  $[1/2J_{12}]$  is shown in Fig.2, where the evolution time  $1/2J_{12}$  is divided into eight identical segments.

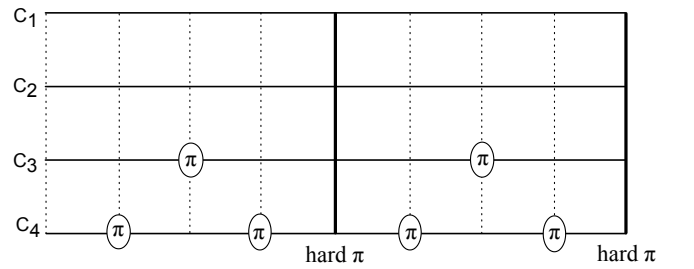


FIG. 2: Refocusing scheme to implement  $[1/2J_{12}]$ . The ellipses represent the strongly modulating  $\pi$  pulses. The evolution time  $1/2J_{12}$  is divided into eight identical segments.

We use Eq. (7) to implement  $U_{zzzz}(T)$  through the pulse sequence

$$\begin{aligned}
& [\frac{\pi}{2}]_x^2 \rightarrow [\pi]_y^2 \rightarrow [\frac{1}{2J_{12}}] \rightarrow [\frac{\pi}{2}]_{-y}^2 \rightarrow [\frac{\pi}{2}]_x^3 \rightarrow [\pi]_y^3 \rightarrow [\frac{1}{2J_{23}}] \rightarrow [\frac{\pi}{2}]_{-y}^3 \rightarrow [\frac{J_{1234}T}{J_{34}}] \\
& \rightarrow [\frac{\pi}{2}]_{-y}^3 \rightarrow [\frac{1}{2J_{23}}] \rightarrow [\frac{\pi}{2}]_{-x}^3 \rightarrow [\frac{\pi}{2}]_{-y}^2 \rightarrow [\frac{1}{2J_{12}}] \rightarrow [\frac{\pi}{2}]_{-x}^2
\end{aligned} \tag{11}$$

where  $[\frac{\pi}{2}]_{-y}^2$  denotes a  $\pi/2$  pulse along  $-y$  axis on C2. The corresponding evolution is  $e^{-i(\pi/4)\sigma_y^2}$ . All spin selective pulses are strongly modulated pulses (SMPs) [11]. A SMP consists of a series of non-selective (hard) pulses that modulate the system's dynamics strongly to produce precisely a desired spin-selective unitary propagator. In our experiments the fidelity of each SMP is larger than 0.99. The total duration time of the whole experiment is about 80 ms.

We choose the state

$$\rho_{ini} = \sigma_x^3, \tag{12}$$

as the initial state, which is prepared by

$$[\frac{\pi}{2}]_y^{1,2,4} \rightarrow [grad]_z \rightarrow [\frac{\pi}{2}]_y^3$$

from the thermal equilibrium [5, 8, 12]. Here we use the deviation density matrix to describe the state of the NMR system [13, 14]. The carbon spectrum for the system in  $\rho_{ini}$  is shown in Fig. 3, where the signals are chosen as the reference signals for the following spectra. The small  $J_{13}$  causes the partial overlapping peaks.

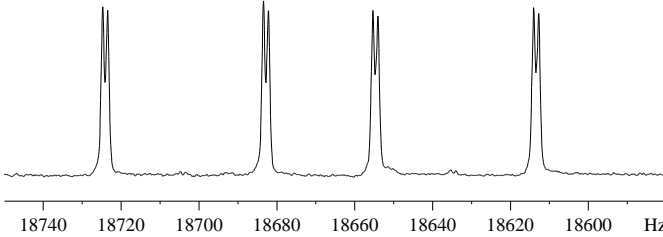


FIG. 3: The C3 spectra when the system lies in  $\rho_{ini} = \sigma_x^3$ .

Under the four-body interaction, the state of this system changes from  $\rho_{ini}$  to

$$\rho_{zzzz}(T) = \sigma_x^3 \cos(\pi J_{1234}T) + \sigma_z^1 \sigma_z^2 \sigma_y^3 \sigma_z^4 \sin(\pi J_{1234}T). \tag{13}$$

When  $\pi J_{1234}T = n\pi/4$  with  $n = 0, 1, \dots, 8$ , the spectra of C3 are shown as Fig. 4. The experimental results agree on the theoretical expectations. By integrating over the eight peaks we obtain the evolution of  $\langle \sigma_x^3 \rangle$  as a function of time,  $\pi J_{1234}T$ , and is shown in Fig. 5. The curve can be fitted as  $\langle \sigma_x^3 \rangle = 1.081 \cos(1.008\pi J_{1234}T)$ , which agrees well with the theoretical expectation  $\langle \sigma_x^3 \rangle = \cos(\pi J_{1234}T)$ . The small discrepancy is due to the imperfection of pulse and decoherence.

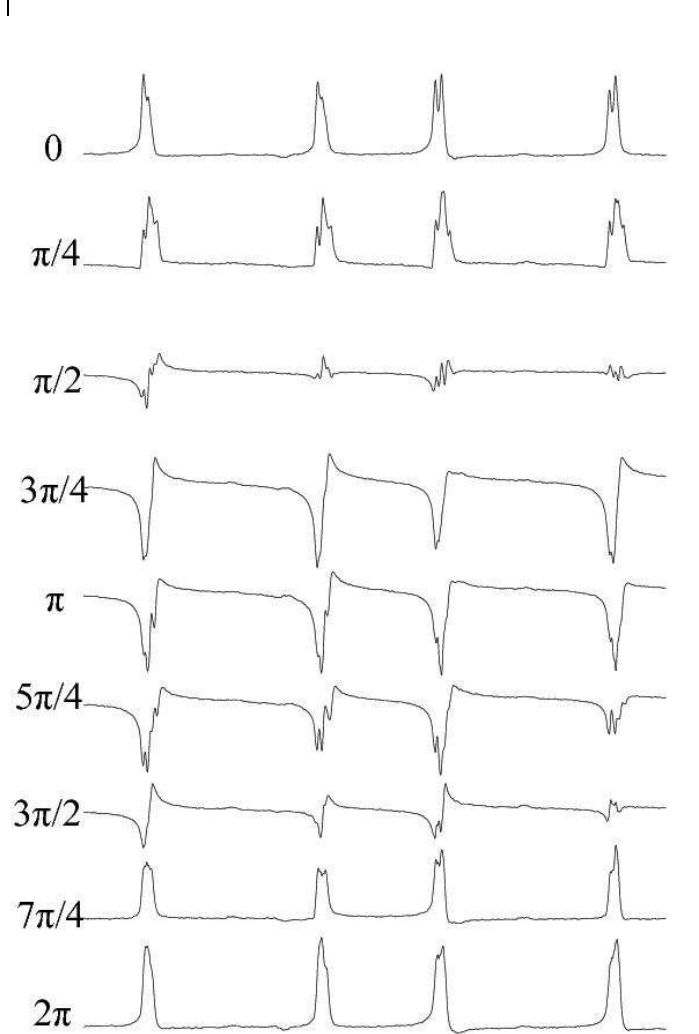


FIG. 4: NMR spectra of C3 in evolution under a four-body interaction. From top to bottom, the figures correspond to  $\pi J_{1234}T = n\pi/4$  with  $n = 0, 1, \dots, 8$ , respectively.

#### IV. SUMMARY

We have experimentally simulated the four-body interaction in a four-qubit NMR quantum information processor. The experiment results show good agreement with the theoretical expectations. The SMP makes the simulation in NMR very well. With this experiment, one

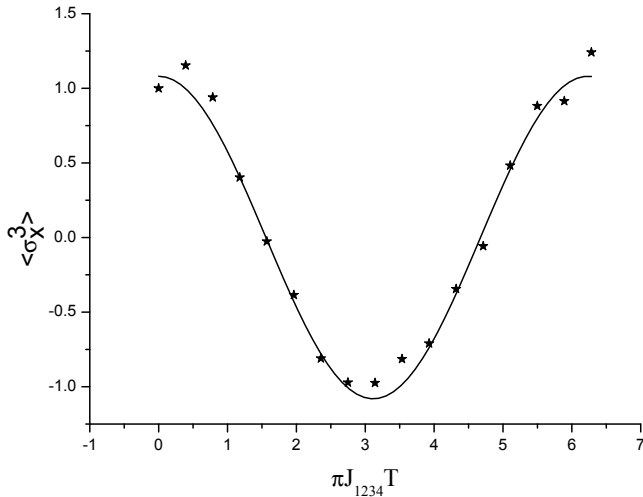


FIG. 5: The expectation value  $\langle \sigma_x^3 \rangle$  versus  $\pi J_{1234} T$  under  $U_{zzzz}$ . The curve can be fitted as  $\langle \sigma_x^3 \rangle = 1.081 \cos(1.008\pi J_{1234} T)$ .

can proceed to demonstrate large quantum system simulations, and look into interesting physical phenomenon such as phase transitions in quantum systems with four-body interaction. The simulation method used here in NMR techniques can be generalized to other Ising type quantum computer.

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